

# Analytical Chemistry

## McElvain Seminar Series



Jimmy K. Eng

Thursday, February 16<sup>th</sup>, 2017  
12:15 pm  
Rm 1315, Chemistry Bldg.

### Algorithms, optimizations, peaks, peptides, and a journey through computational proteomics

Peptide and protein identification remains one of the most widely used applications in mass spectrometry analysis. This talk will present a history into the development of the SEQUEST algorithm and discuss how design changes and algorithm optimizations allow it to remain as relevant today as it was when it was first developed in the early 90s. Now with one variant as an open source project, the latest developments in the Comet MS/MS search tool will be presented.

Additionally, Mr. Eng's recent collaborative work with cross-linking identifications will be discussed. We'll dive into issues related to validating identified cross-links and present the development of a new cross-link search tool.

*UWPR Senior Software Engineer  
Developer of SEQUEST*

